U.S. DEPARTMENT OF COMMERCE
Patent and Trademark Office

SEARCH REQUEST FORM

4-45

Requestor's Name: Mark Clardy Serial Number: 08/537,843

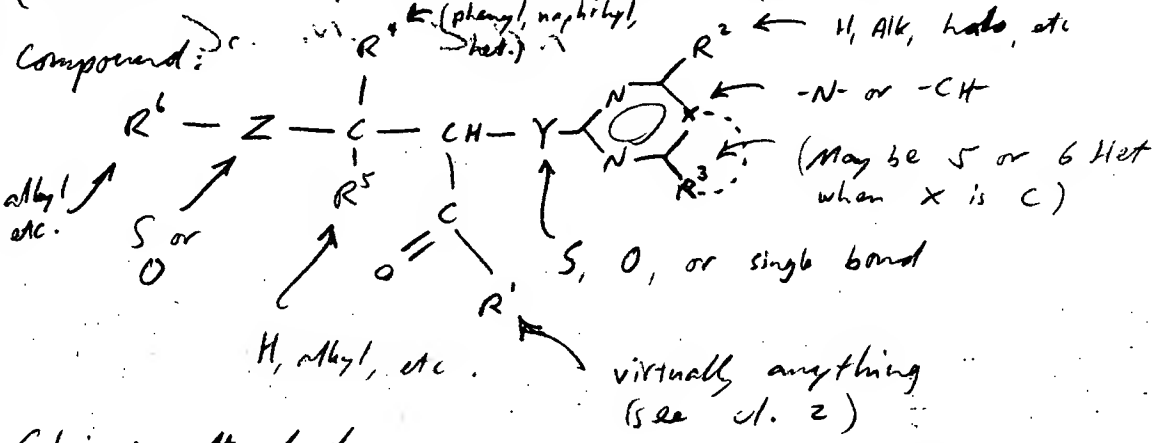
Date: 8/26/96 Phone: ? Art Unit: _____

Search Topic:

Please write a detailed statement of search topic. Describe specifically as possible the subject matter to be searched. Define any terms that may have a special meaning. Give examples or relevant citations, authors keywords, etc., if known. For sequences, please attach a copy of the sequence. You may include a copy of the broadest and/or most relevant claim(s).

(Herbicidal) Compound / Composition / Method.

Compound:

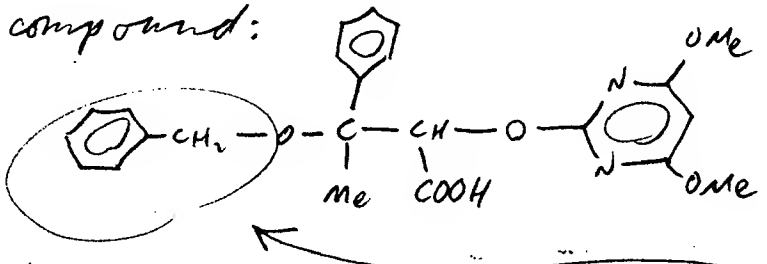


Claims attached

Face of file attached.

All refs are P.D. (or later & same inv.)

Tested compound:



prior art (EP-A 409 368) has methyl instead of benzyl here

19

STAFF USE ONLY

Date completed: Alex 9-5-96
Searcher: _____
Terminal time: _____
Elapsed time: _____
CPU time: _____
Total time: _____
Number of Searches: _____
Number of Databases: _____

Search Site
_____ STIC
__X__ CM-1
_____ Pre-S

Type of Search
_____ N.A. Sequence
_____ A.A. Sequence
_____ Structure
_____ Bibliographic

Vendors
_____ IG Suite
__X__ STN
_____ Dialog
_____ APS
_____ Geninfo
_____ SDC
_____ DARC/Questel
_____ Other

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=> d his

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L1              STR
L2          190 SEA FILE=REGISTRY SSS FUL L1
               ---------
                ACT CLARDY2/A
               ---------
L3              STR
L4   (      190)SEA FILE=REGISTRY SSS FUL L3
L5              STR
L6           17 SEA FILE=REGISTRY SUB=L4 SSS FUL L5
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L7           11 S L2
L8            2 S L6
L9            9 S L7 NOT L8

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FILE 'REGISTRY' ENTERED AT 07:42:15 ON 05 SEP 96
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 1996 American Chemical Society (ACS)

STRUCTURE FILE UPDATES:  02 SEPT 96  HIGHEST RN 180310-23-0
DICTIONARY FILE UPDATES: 04 SEPT 96  HIGHEST RN 180310-23-0

TSCA INFORMATION NOW CURRENT THROUGH DECEMBER 1995

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

=> d his l1-16

     (FILE 'REGISTRY' ENTERED AT 07:29:37 ON 05 SEP 96)
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L2          190 SEA FILE=REGISTRY SSS FUL L1
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L4   (      190)SEA FILE=REGISTRY SSS FUL L3
L5              STR
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broad search

L6 17 SEA FILE=REGISTRY SUB=L4 SSS FUL L5 tested compound

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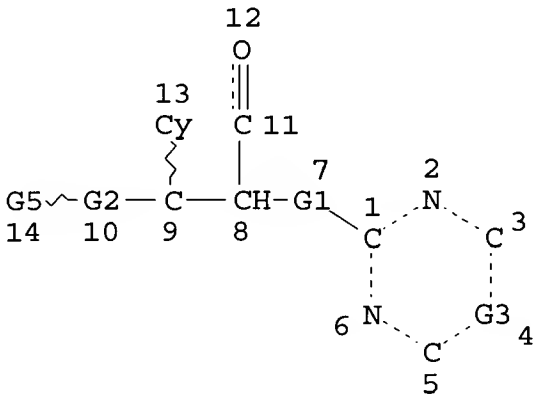
L1 STR



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VAR G3=N/C
VAR G5=C/CB
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE
L2 190 SEA FILE=REGISTRY SSS FUL L1

100.0% PROCESSED 62595 ITERATIONS 190 ANSWERS
SEARCH TIME: 00.01.06

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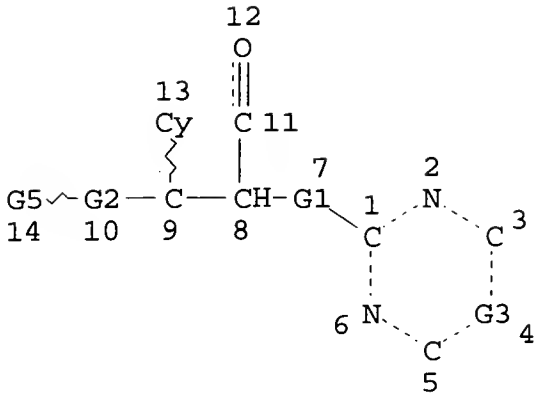

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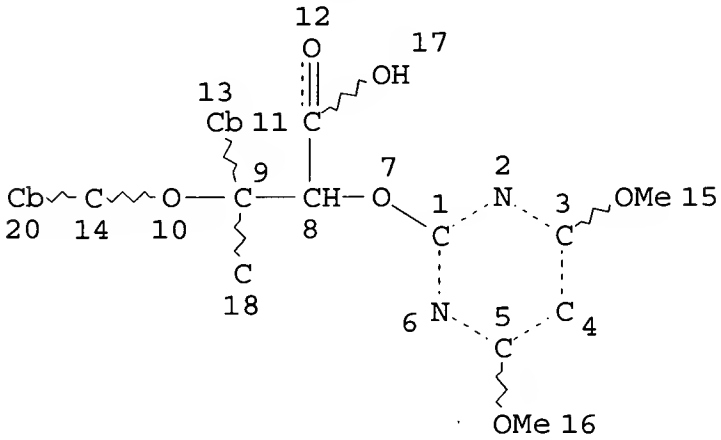

NODE ATTRIBUTES:
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DEFAULT ECLEVEL IS LIMITED

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NUMBER OF NODES IS 19

STEREO ATTRIBUTES: NONE
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SEARCH TIME: 00.00.03

=> fil hcaplus
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USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 1996 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1967 - 5 Sep 1996 VOL 125 ISS 11
FILE LAST UPDATED: 5 Sep 1996 (960905/ED)

Meeting Abstracts for Orlando ACS Meeting Now in HCAPLUS. Please see NEWS for details.
'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

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'HISL' IS NOT A VALID FORMAT FOR FILE 'HCAPLUS'
'L7-' IS NOT A VALID FORMAT FOR FILE 'HCAPLUS'
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(FILE 'REGISTRY' ENTERED AT 07:29:37 ON 05 SEP 96)

FILE 'HCAPLUS' ENTERED AT 07:41:52 ON 05 SEP 96
L7 11 S L2
L8 2 S L6 narrower struct.
L9 9 S L7 NOT L8 broad struct

FILE 'REGISTRY' ENTERED AT 07:42:15 ON 05 SEP 96

FILE 'HCAPLUS' ENTERED AT 07:42:27 ON 05 SEP 96

=> d all l8 1-2

L8 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 1996 ACS
AN 1995:916669 HCAPLUS
DN 123:307319

TI Carboxylic acid derivatives as inhibitors of endothelin binding to receptors Inv.

IN Baumann, Ernst; Vogelbacher, Uwe Josef; Rheinheimer, Joachm; Klinge, Dagmar; Riechers, Hartmut; Kroeger, Burkhard; Bialojan, Siegfried; Bollschweiler, Claus; Wernet, Wolfgang; et al.
PA BASF A.-G., Germany

SO Ger. Offen., 31 pp.
CODEN: GWXXBX
PI DE 4411225 A1 951005
AI DE 94-4411225 940331
DT Patent
LA German
IC ICM A61K031-505
ICS A61K031-53
CC 2-10 (Mammalian Hormones)
Section cross-reference(s): 34
OS MARPAT 123:307319

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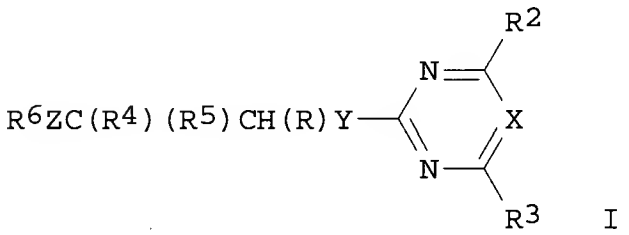

I

AB Carboxylic acid derivs. I [R = CHO, CO2H, group hydrolyzable to CO2H; R2, R3 = halo, C1-4 alkyl, C1-4 alkoxy, C1-4 haloalkoxy, C1-4 alkylthio; X = N, CR14; R4 = (substituted) C1-10 alkyl, (substituted) C3-12 cycloalkyl or cycloalkenyl, (substituted) C3-6 alkenyl or alkynyl, (substituted) heterocyclyl, (substituted) Ph or naphthyl; R5 = H, (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, or R4 and R5 complete a 3-8-membered ring; R6 = (substituted) alkyl, (substituted) alkenyl, (substituted) alkynyl, (substituted) cycloalkyl; R14 = H or forms an O-contg. 3-4-membered alkylene or alkenylene chain with R3; Y = S, O, single bond; Z = S, O] are prepd. as inhibitors of endothelin binding to receptors for treatment of e.g. (pulmonary) hypertension, acute myocardial infarct, Raynaud's syndrome, atherosclerosis, and asthma. Thus, I (R1 = CO2H, R2 = R3 = OMe, R4 = Ph, R5 = Me, R6 = 4-isopropylphenyl, X = CH, Y = Z = O) inhibited binding of endothelin to endothelin A receptors of cloned human CHO cells and endothelin B receptors of guinea pig cerebellar membranes with Ki 2.5 .times. 10-7 and 3.0 .times. 10-6M, resp. I (R = CO2Me, R2 = R3 = OMe, R4 = R6 = Ph, R5 = H, X = CH, Y = S, Z = O) was prepd. by reaction of Me

3-phenoxy-3-phenyl-2-hydroxybutyrate (prepn. given) with MeSO2Cl and 4,6-dimethoxypyrimidine-2-thiol.

ST pyrimidinylalkanecarboxylate prepn endothelin receptor inhibitor

IT Antihypertensives
Vasodilators
(carboxylic acid derivs. as inhibitors of endothelin binding to receptors)

IT Receptors
RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
(ETA (endothelin, A), carboxylic acid derivs. as inhibitors of endothelin binding to receptors)

IT Blood vessel, disease
(Raynaud's phenomenon, carboxylic acid derivs. as inhibitors of endothelin binding to receptors)

IT Bronchodilators
(antiasthmatics, carboxylic acid derivs. as inhibitors of endothelin binding to receptors)

IT Antiarteriosclerotics
(antiatherosclerotics, carboxylic acid derivs. as inhibitors of endothelin binding to receptors)

IT Antihypertensives
(pulmonary, carboxylic acid derivs. as inhibitors of endothelin binding to receptors)

IT 123626-67-5, Endothelin 1
RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)
(carboxylic acid derivs. as inhibitors of endothelin binding to receptors)

IT 170296-15-8P
RL: BAC (Biological activity or effector, except adverse); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(carboxylic acid derivs. as inhibitors of endothelin binding to receptors)

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159308-14-2P 159308-15-3P 159308-16-4P 159308-17-5P
159308-18-6P 159308-19-7P 159559-14-5P 159559-15-6P
170296-16-9P 170296-17-0P 170296-18-1P 170296-19-2P
170296-20-5P 170296-21-6P 170296-22-7P 170296-23-8P
170296-24-9P 170296-25-0P 170296-26-1P 170296-27-2P
170296-28-3P 170296-29-4P 170296-30-7P 170296-31-8P
170296-32-9P 170296-33-0P 170296-34-1P 170296-35-2P
170296-36-3P 170296-37-4P 170296-38-5P 170296-39-6P
170296-40-9P 170296-41-0P **170296-42-1P** 170296-43-2P
170296-44-3P 170296-45-4P **170296-46-5P**
170296-47-6P **170296-48-7P** 170296-49-8P

170296-50-1P 170296-51-2P **170296-52-3P**
170296-53-4P **170296-54-5P** 170296-55-6P 170296-56-7P
170296-57-8P 170296-58-9P 170296-59-0P **170296-60-3P**
170296-61-4P 170296-62-5P 170296-63-6P 170296-64-7P
170296-65-8P 170296-66-9P 170296-67-0P 170296-68-1P
170296-69-2P 170296-70-5P 170296-71-6P **170296-72-7P**
170296-73-8P 170296-74-9P 170296-75-0P 170296-76-1P
170296-77-2P 170296-78-3P **170296-79-4P**
170296-80-7P **170296-81-8P 170296-82-9P**
170296-83-0P 170296-84-1P 170296-85-2P 170296-86-3P
170296-87-4P 170296-88-5P 170296-89-6P 170296-90-9P
170296-91-0P 170296-92-1P 170296-93-2P 170296-94-3P
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170297-03-7P 170297-04-8P 170297-05-9P 170297-06-0P
170297-07-1P 170297-08-2P 170297-09-3P 170297-10-6P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(carboxylic acid derivs. as inhibitors of endothelin binding to receptors)

IT 95-48-7, reactions 99-89-8, 4-Isopropylphenol 100-51-6, Benzenemethanol, reactions 106-41-2, 4-Bromophenol 106-44-5, reactions 108-39-4, reactions 108-95-2, Phenol, reactions 371-41-5, 4-Fluorophenol 372-20-3, 3-Fluorophenol 459-56-3, 4-Fluorobenzyl alcohol 5441-04-3 57235-35-5, 4,6-Dimethoxypyrimidine-2-thiol 99334-01-7 113583-35-0, 4,6-Dimethoxy-2-methylsulfonylpyrimidine 159559-29-2 159559-91-8
170297-20-8 170297-29-7 170297-30-0 170297-31-1 170297-32-2
170297-33-3 170297-34-4 170297-35-5 170297-36-6 170297-37-7
170297-38-8 170297-39-9 170297-40-2 170297-41-3 170297-42-4
170297-43-5 170297-44-6
RL: RCT (Reactant)
(carboxylic acid derivs. as inhibitors of endothelin binding to receptors)

IT 159307-92-3P 159307-93-4P 159307-94-5P 159307-95-6P
159307-96-7P 159307-97-8P 159307-98-9P 159307-99-0P
159308-00-6P 159308-01-7P 170297-11-7P 170297-12-8P
170297-13-9P 170297-14-0P 170297-15-1P 170297-16-2P
170297-17-3P 170297-18-4P 170297-19-5P 170297-21-9P
170297-22-0P 170297-23-1P 170297-24-2P 170297-25-3P
170297-26-4P 170297-27-5P 170297-28-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(carboxylic acid derivs. as inhibitors of endothelin binding to receptors)

L8 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 1996 ACS
AN 1995:234868 HCAPLUS
DN 122:31550

TI Preparation of 3-(hetero)arylcarboxylic acid-derivative herbicides with increased species selectivity

IN Baumann, Ernst; Rheinheimer, Joachim; Vogelbacher, Uwe Josef; Bratz, Matthias; Theobald, Hans; Gerber, Matthias; Walter, Helmut; Rademacher, Wilhelm; Westphalen, Karl Otto

PA BASF A.-G., Germany

SO Ger. Offen., 25 pp.
CODEN: GWXXBX

PI DE 4313412 A1 941027

AI DE 93-4313412 930423

DT Patent

LA German

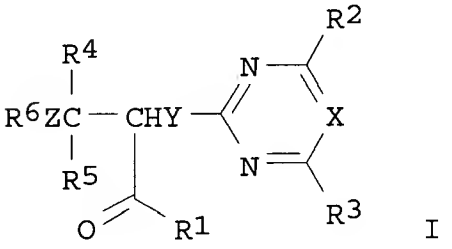
IC ICM C07D239-60
ICS C07D401-12; C07C069-66; C07C309-65; C07C309-73; C07D403-12; C07D405-12; C07D409-12; C07D413-12; C07D417-12; C07D491-048; A01N043-54

ICA C07D521-00; C07D251-12; C07D307-54; C07D333-24; C07D213-55; C07D277-30; C07D261-08; C07D233-64

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 5

OS MARPAT 122:31550

GI



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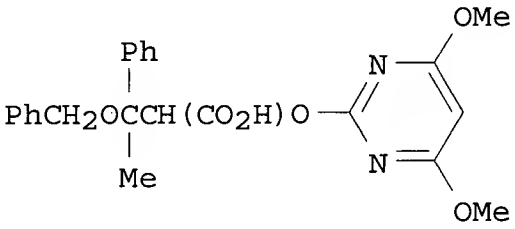

II

AB The title compds. [I; R1 = H, succinylimidoxy, (un)substituted N-contg. 5-member heterocyclic group, etc.; R2, R3 = halogen, C1-4 alkyl or alkoxy or alkylthio, etc.; R4 = (un)substituted Ph, (un)substituted naphthyl, (un)substituted heteroarom. residue, etc.; R5 = H, alkyl, alkenyl, alkynyl, cycloalkyl, Ph, etc.; R6 = (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl; X = N, (un)substituted CH; Y = direct bond, O, S; Z = O, S], useful as herbicides which have reduced toxicity com. plant species, are prepd. Thus, pyrimidine deriv. II (m.p. 165.degree.; decompn.) was prepd. and demonstrated 10% plant loss when applied to Gossypium hirsutum (i.e., cotton) at 0.125 kg/ha, vs. 35% plant loss for a control expt. using I (R1 = OH, R2 = R3 = OMe, R4 = Ph, R5 = R6 = Me, X= CH, Y = Z = O).

ST selective herbicide prepn pyrimidinylalkylcarboxylic acid;

heteroarylcarboxylic acid deriv herbicide
IT Herbicides
(3-(hetero)arylcarboxylic acids)
IT 159559-10-1P
RL: AGR (Agricultural use); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 3-(hetero)arylcarboxylic acid-deriv. herbicides with increased species selectivity)
IT 159559-01-0P 159559-02-1P 159559-03-2P 159559-04-3P
159559-05-4P 159559-06-5P 159559-07-6P 159559-08-7P
159559-09-8P **159559-11-2P** 159559-12-3P 159559-13-4P
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RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 3-(hetero)arylcarboxylic acid-deriv. herbicides with increased species selectivity)
IT 100-51-6, Benzyl alcohol, reactions 5441-04-3 113583-35-0,
4,6-Dimethoxy-2-methylsulfonylpyrimidine 159559-29-2
RL: RCT (Reactant)
(prepn. of 3-(hetero)arylcarboxylic acid-deriv. herbicides with increased species selectivity)

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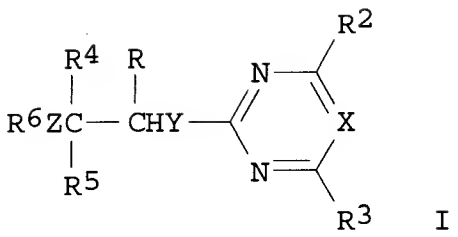
E33 THROUGH E49 ASSIGNED

=> d .ca l9 1-9

L9 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 1996 ACS
AN 1996:401554 HCAPLUS
DN 125:58534
TI Preparation of pyrimidine- and triazine-derivative endothelin receptor antagonists
IN Riechers, Hartmut; Klinge, Dagmar; Amberg, Wilhelm; Kling, Andreas; Mueller, Stefan; Baumann, Ernst; Rheinheimer, Joachim; Vogelbacher, Uwe Josef; Wernet, Wolfgang; et al.
PA BASF A.-G., Germany
SO Ger. Offen., 28 pp.
CODEN: GWXXBX
PI DE 19533023 A1 960418
AI DE 95-19533023 950907
PRAI DE 94-4436851 941014
DT Patent
LA German
OS MARPAT 125:58534
GI



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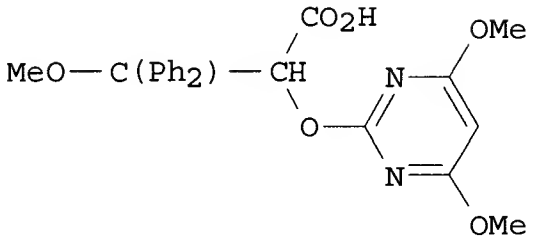


II

AB The title compds. [I; R = CHO, tetrazolyl, CN, CO2H, groups cleavable to CO2H; R2 = (un)substituted NH2, halogen, (un)substituted alkyl, etc.; R3 = H, OH, (un)substituted NH2, halogen, (un)substituted alkyl, etc.; R4, R5 = (un)substituted Ph or naphthyl; R6 = H, alkyl, alkenyl, alkynyl, alkylcarbonyl, (un)substituted Ph, etc.; X = N, (un)substituted CH; Y = direct bond, S, O; Z = S, O, SO, SO2, direct bond], useful as endothelin receptor antagonists, are prepd. Thus, pyrimidine deriv. II, m.p. 167.degree., demonstrated a Ki ETA of 6 nM.

IT **178306-68-8P**
RL: BAC (Biological activity or effector, except adverse); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of pyrimidine- and triazine-deriv. endothelin receptor antagonists)

IT **177036-81-6P 177036-86-1P 177036-87-2P**
178306-45-1P 178306-46-2P 178306-57-5P
178306-58-6P 178306-59-7P 178306-60-0P
178306-61-1P 178306-64-4P 178306-65-5P
178306-66-6P 178306-67-7P 178306-69-9P
178306-70-2P 178306-71-3P 178306-72-4P
178306-73-5P 178306-74-6P 178306-75-7P
178306-76-8P 178306-77-9P 178306-78-0P
178306-79-1P 178306-80-4P 178306-81-5P
178306-82-6P 178306-83-7P 178306-84-8P
178306-85-9P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of pyrimidine- and triazine-deriv. endothelin receptor antagonists)

IC ICM C07D239-60
ICS C07D239-70; C07D403-12; C07D405-12; C07D491-044; C07D487-04; C07D495-04; C07D409-12; C07D413-12; C07D417-12; A61K031-41;

A61K031-505
ICA C07D521-00
ICI C07M007-00; C07D491-044, C07D239-00, C07D315-00; C07D487-04, C07D239-00, C07D209-00
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
IT **178306-68-8P**
RL: BAC (Biological activity or effector, except adverse); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of pyrimidine- and triazine-deriv. endothelin receptor antagonists)
IT **177036-81-6P 177036-86-1P 177036-87-2P**
177037-02-4P **178306-45-1P 178306-46-2P**
178306-57-5P 178306-58-6P 178306-59-7P
178306-60-0P 178306-61-1P 178306-62-2P
178306-63-3P **178306-64-4P 178306-65-5P**
178306-66-6P 178306-67-7P 178306-69-9P
178306-70-2P 178306-71-3P 178306-72-4P
178306-73-5P 178306-74-6P 178306-75-7P
178306-76-8P 178306-77-9P 178306-78-0P
178306-79-1P 178306-80-4P 178306-81-5P
178306-82-6P 178306-83-7P 178306-84-8P
178306-85-9P 178306-86-0P 178306-87-1P 178306-88-2P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of pyrimidine- and triazine-deriv. endothelin receptor antagonists)

L9 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 1996 ACS
AN 1996:271791 HCAPLUS
DN 125:328
TI Discovery and Optimization of a Novel Class of Orally Active Nonpeptidic Endothelin-A Receptor Antagonists
AU Riechers, Hartmut; Albrecht, Hans-Peter; Amberg, Willi; Baumann, Ernst; Bernard, Harald; Boehm, Hans-Joachim; Klinge, Dagmar; Kling, Andreas; Mueller, Stefan; et al.
CS Hauptlaboratorium, BASF AG, Ludwigshafen, 67056, Germany
SO J. Med. Chem. (1996), 39(11), 2123-8
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
OS CASREACT 125:328; CJACS-IMAGE; CJACS
AB A novel class of endothelin-A receptor ligands was discovered by high-throughput screening. Lead structure optimization led to highly potent antagonists which can be synthesized in a short sequence. The compds. are endothelin-A-selective, are orally available, and show a long duration of action.

IT **171714-84-4P**, LU 127043 **177036-81-6P**
177036-82-7P 177036-83-8P 177036-84-9P
177036-85-0P 177036-86-1P 177036-87-2P
177036-88-3P 177036-89-4P 177036-90-7P
177036-91-8P 177036-93-0P 177036-94-1P
177036-95-2P, LU 134981 **177036-96-3P**, LU 136181
177036-97-4P 177036-98-5P 177036-99-6P
177037-00-2P
RL: BAC (Biological activity or effector, except adverse); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of a novel class of orally active nonpeptidic endothelin-a receptor antagonists)

IT **159308-17-5**, LU 110896 **170297-04-8**, LU 110897
RL: BAC (Biological activity or effector, except adverse); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(prepn. of a novel class of orally active nonpeptidic endothelin-a receptor antagonists)

IT **177037-01-3**
RL: RCT (Reactant)
(prepn. of a novel class of orally active nonpeptidic endothelin-a receptor antagonists)

IT **177036-79-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of a novel class of orally active nonpeptidic endothelin-a receptor antagonists)

CC 1-3 (Pharmacology)
Section cross-reference(s): 2, 28

IT **171714-84-4P**, LU 127043 **177036-81-6P**
177036-82-7P 177036-83-8P 177036-84-9P
177036-85-0P 177036-86-1P 177036-87-2P
177036-88-3P 177036-89-4P 177036-90-7P
177036-91-8P 177036-92-9P **177036-93-0P**
177036-94-1P 177036-95-2P, LU 134981
177036-96-3P, LU 136181 **177036-97-4P**
177036-98-5P 177036-99-6P 177037-00-2P
RL: BAC (Biological activity or effector, except adverse); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of a novel class of orally active nonpeptidic endothelin-a receptor antagonists)

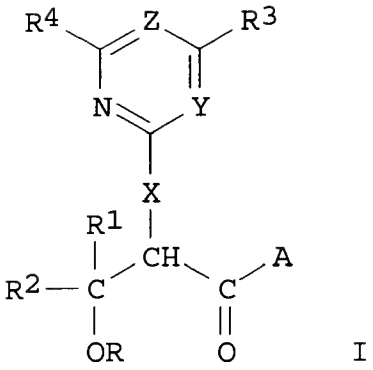
IT **159308-17-5**, LU 110896 **170297-04-8**, LU 110897
RL: BAC (Biological activity or effector, except adverse); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(prepn. of a novel class of orally active nonpeptidic endothelin-a receptor antagonists)

IT 90-98-2, 4,4'-Dichlorobenzophenone 96-34-4, Chloroacetic acid

methyl ester 119-61-9, Benzophenone, reactions 345-70-0, 3,3'-Difluorobenzophenone 345-92-6, 4,4'-Difluorobenzophenone 393-52-2, 2-Fluorobenzoyl chloride 591-17-3, 3-Bromotoluene 611-97-2, 4,4'-Dimethylbenzophenone 1072-85-1, 2-Fluorobromobenzene 1711-05-3, 3-Methoxybenzoic acid chloride 1711-06-4, 3-Methylbenzoyl chloride 2398-37-0, 3-Methoxybromobenzene 35144-22-0, 2-(Methylsulfonyl)-4,6-dimethylpyrimidine 57268-32-3 77166-01-9 113583-35-0, 2-(Methylsulfonyl)-4,6-dimethoxypyrimidine 143323-12-0 149228-24-0 **177037-01-3** 177037-02-4 177037-03-5
RL: RCT (Reactant)
(prepn. of a novel class of orally active nonpeptidic endothelin-a receptor antagonists)

IT 2852-68-8P, 3,3'-Dimethylbenzophenone 39193-85-6P, 3,3'-Dimethoxybenzophenone 76527-25-8P 177036-78-1P **177036-79-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of a novel class of orally active nonpeptidic endothelin-a receptor antagonists)

L9 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 1996 ACS
AN 1996:237460 HCAPLUS
DN 124:289560
TI Preparation of pyrimidinyl- and triazinyl-oxy and thio-3-haloalkyl-propionic acid derivatives as herbicides
IN Luethy, Christoph; Lutz, William
PA Ciba-Geigy A.-G., Switz.
SO PCT Int. Appl., 115 pp.
CODEN: PIXXD2
PI WO 9600219 A1 960104
DS W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TT, UA, US, UZ, VN
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG
AI WO 95-EP2295 950613
PRAI CH 94-2045 940627
CH 94-2858 940920
DT Patent
LA English
OS MARPAT 124:289560
GI



I

AB The title compds. [I; A = alkylthio, alkyloxy, OH, (un)substituted heterocyclyl, etc.; R = H, (un)substituted alkyl, haloalkyl, (un)substituted Ph, etc.; R1 = C1-7 haloalkyl; R2 = H, alkyl, alkenyl, cycloalkyl, (un)substituted Ph, pyridyl, thienyl, etc.; R3 = Me, Et, MeO, EtO, CF3O, HCF2O, etc.; R4 = F, Cl, Me, Et, Pr, cyclopropyl, MeO, EtO, etc; X = O, S; Y = N or if Z = N then Y is N, (un)substituted CH; Z = N, (un)substituted CH], useful as selective herbicides esp. for controlling weeds, are prepd. and I-contg. formulations presented. Thus, I (A = OCMe3, R = R2 = Me, R3 = R4 = OMe, X = S, Y = N, Z = CH) was prepd.

IT **175527-71-6P 175527-72-7P**
RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of pyrimidinyl- and triazinyl-oxy and thio-3-haloalkyl-propionic acid derivs. as herbicides)

IC ICM C07D239-60
ICS A01N043-40; C07D405-12; C07D401-00; C07D233-54; C07D401-12

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 5

IT 161600-98-2P 164790-07-2P 175527-30-7P 175527-31-8P
175527-36-3P 175527-37-4P 175527-38-5P 175527-39-6P
175527-40-9P 175527-41-0P 175527-42-1P 175527-43-2P
175527-44-3P 175527-45-4P 175527-46-5P 175527-47-6P
175527-48-7P 175527-49-8P 175527-50-1P 175527-51-2P
175527-52-3P 175527-53-4P 175527-54-5P 175527-55-6P
175527-56-7P 175527-57-8P 175527-58-9P 175527-59-0P
175527-60-3P 175527-61-4P 175527-62-5P 175527-63-6P
175527-64-7P 175527-65-8P 175527-66-9P 175527-67-0P
175527-68-1P 175527-69-2P 175527-70-5P **175527-71-6P**
175527-72-7P 175527-73-8P 175527-74-9P 175527-75-0P
175527-76-1P 175527-77-2P 175527-78-3P 175527-79-4P
175527-80-7P 175527-81-8P 175527-82-9P 175527-83-0P
175527-84-1P 175527-85-2P 175527-86-3P 175527-87-4P

175527-88-5P 175527-89-6P 175527-90-9P 175527-91-0P
175527-92-1P 175527-93-2P 175527-94-3P 175527-95-4P
175527-96-5P 175527-97-6P 175527-98-7P 175527-99-8P
175528-00-4P 175528-01-5P 175528-02-6P 175528-03-7P
175528-04-8P 175528-05-9P 175528-06-0P 175528-07-1P
175528-08-2P 175528-09-3P 175528-10-6P 175528-11-7P
175528-12-8P 175528-13-9P 175528-14-0P 175528-15-1P
175528-16-2P 175528-17-3P 175528-18-4P 175528-19-5P
175528-20-8P 175528-21-9P 175528-22-0P 175528-23-1P
175528-24-2P 175528-25-3P 175528-26-4P 175528-27-5P
175528-28-6P 175528-29-7P 175528-30-0P 175528-31-1P
175528-32-2P 175528-33-3P 175528-34-4P 175528-35-5P
175528-36-6P 175528-37-7P 175528-38-8P 175528-39-9P
175528-40-2P 175528-41-3P 175528-42-4P 175528-43-5P
175528-44-6P 175528-45-7P 175528-46-8P 175528-47-9P
175528-48-0P 175528-49-1P 175528-50-4P 175528-51-5P
175528-52-6P 175528-53-7P 175528-54-8P 175528-55-9P
175528-56-0P 175528-57-1P 175528-58-2P 175528-59-3P
175528-60-6P 175528-61-7P 175528-62-8P 175528-63-9P
175528-64-0P 175528-65-1P 175528-66-2P 175528-67-3P
175528-68-4P 175528-69-5P 175528-70-8P 175528-71-9P
175528-72-0P 175528-73-1P 175528-74-2P 175528-75-3P
175528-76-4P 175528-77-5P 175528-78-6P 175528-79-7P
175528-80-0P 175528-81-1P 175672-08-9P 175672-09-0P
175672-10-3P 175672-11-4P 175672-12-5P 175672-13-6P
175672-14-7P 175672-15-8P 175672-16-9P 175672-17-0P
175672-18-1P 175672-19-2P
RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of pyrimidinyl- and triazinyl-oxy and thio-3-haloalkyl-propionic acid derivs. as herbicides)

L9 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 1996 ACS
AN 1995:966284 HCAPLUS
DN 124:22417
TI Receptor selectivity of endothelin antagonists and prevention of vasoconstriction and endothelin-induced sudden death
AU Raschack, Manfred; Unger, Liliane; Riechers, Hartmut; Klinge, Dagmar
CS Knoll AG, Ludwigshafen, Germany
SO J. Cardiovasc. Pharmacol. (1995), 26(Suppl. 3), S397-S399
CODEN: JCPCDT; ISSN: 0160-2446
DT Journal
LA English
AB The new endothelin (ET) receptor antagonist LU 127043 shows higher ETA affinity than BQ 123, Ro 46 2005, and BMS 182874, with a Ki of 6 nmol/L vs. 19, 28, and 57 nmol/L. ETA/ETB selectivity of LU 127043 of about 160 is comparable to that of BQ 123 (200) and is much greater than that of Ro 46-2005 (0.93) and SB 209670 (0.74). In rabbit aortic segments, LU 127043 showed Et antagonistic potency

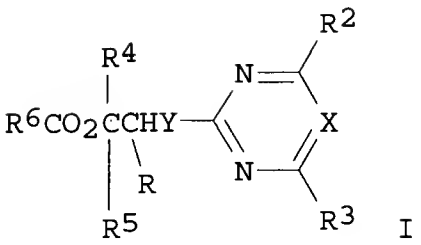
similar to that of BQ 123 and BMS 182874 (pA2 7.34 vs. 7.36 and 7.09), whereas SB 209670 is more potent (9.80). In rats, LU 127043 completely prevents the ET-1-induced sudden death due to coronary constriction, as indicated by a pronounced T-wave increase. With i.v. pretreatment, LU 127043 is as selective as SB 209670, whereas it is three times more active using 4 h oral pretreatment. Even 8 h after oral administration, LU 127043, in contrast to SB 209670, provides dose-dependent protection. Hence, LU 127043 is an example of a selective ETA antagonist with high oral availability and long duration of action. Because the in vivo efficacy of other high affinity ET antagonists is relatively low, further optimization for therapeutic use should conc. on pharmacokinetic properties.

IT **171714-84-4**, LU 127043
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BIOL (Biological study); PROC (Process)
(receptor selectivity of endothelin antagonists and prevention of vasoconstriction and endothelin-induced sudden death)

CC 2-10 (Mammalian Hormones)

IT 136553-81-6, BQ 123 150725-87-4, Ro 46-2005 153042-42-3, BMS 182874 157659-79-5, SB 209670 **171714-84-4**, LU 127043
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BIOL (Biological study); PROC (Process)
(receptor selectivity of endothelin antagonists and prevention of vasoconstriction and endothelin-induced sudden death)

L9 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 1996 ACS
AN 1995:667255 HCAPLUS
DN 123:83384
TI Preparation of 3-hydroxycarboxylic acid-derivative herbicides and plant-growth regulators
IN Baumann, Ernst; Rheinheimer, Joachim; Vogelbacher, Uwe Josef; Gerber, Matthias; Rademacher, Wilhelm; Walter, Helmut; Westphalen, Karl-Otto
PA BASF A.-G., Germany
SO Ger. Offen., 26 pp.
CODEN: GWXXBX
PI DE 4335950 A1 950427
AI DE 93-4335950 931021
DT Patent
LA German
OS MARPAT 123:83384
GI



I

AB The title compds. [I; R = CHO, CO2H, CO2H substituted with a hydrolyzable group; R2, R3 = halogen, (un)substituted alkyl, (un)substituted alkoxy, alkylthio; R4 = (un)substituted alkyl; R5 = H, alkyl, alkenyl, alkynyl, alkylcarbonyl, cycloalkyl, (un)substituted Ph, etc.; R6 = (un)substituted alkyl; X = N, (un)substituted CH; Y = O, S] [e.g., Me 3-acetoxy-3-phenyl-2-[(4,6-dimethoxypyrimidin-2-yl)thio]butyrate], useful as herbicides and plant-growth regulators (no data), are prepd.

IT **164790-06-1P**
RL: AGR (Agricultural use); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 3-hydroxycarboxylic acid-deriv. herbicides and plant-growth regulators)

IT **164790-03-8P**
RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 3-hydroxycarboxylic acid-deriv. herbicides and plant-growth regulators)

IC ICM C07D239-46
ICS C07D251-30; C07D401-12; C07D405-12; C07D409-12; C07D411-12; C07D413-12; C07D417-12; A01N043-54; A01N043-66; A01N043-74; A01N043-56

ICI C07D401-12, C07D213-06; C07D251-30; C07D405-12, C07D307-06; C07D239-46; C07D409-12, C07D333-06

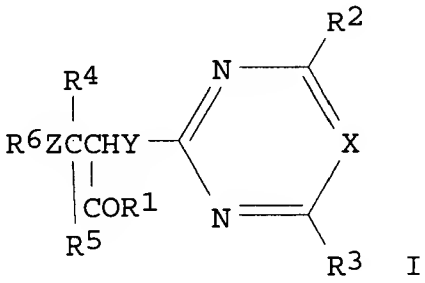
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 5

IT **164790-06-1P** 164790-07-2P
RL: AGR (Agricultural use); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 3-hydroxycarboxylic acid-deriv. herbicides and plant-growth regulators)

IT **164790-03-8P** 164790-04-9P 164790-05-0P 164790-09-4P
RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 3-hydroxycarboxylic acid-deriv. herbicides and

plant-growth regulators)

L9 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 1996 ACS
AN 1994:700921 HCAPLUS
DN 121:300921
TI Preparation of 3-(hetero)aryloxy(thio)carboxylic acid derivatives as agrochemical herbicides
IN Baumann, Ernst; Rheinheimer, Joachim; Vogelbacher, Uwe Josef; Bratz, Matthias; Meyer, Norbert; Gerber, Matthias; Walter, Helmut; Rademacher, Wilhelm; Westphalen, Karl Otto
PA BASF A.-G., Germany
SO Ger. Offen., 26 pp.
CODEN: GWXXBX
PI DE 4313413 A1 941027
AI DE 93-4313413 930423
DT Patent
LA German
OS MARPAT 121:300921
GI



I

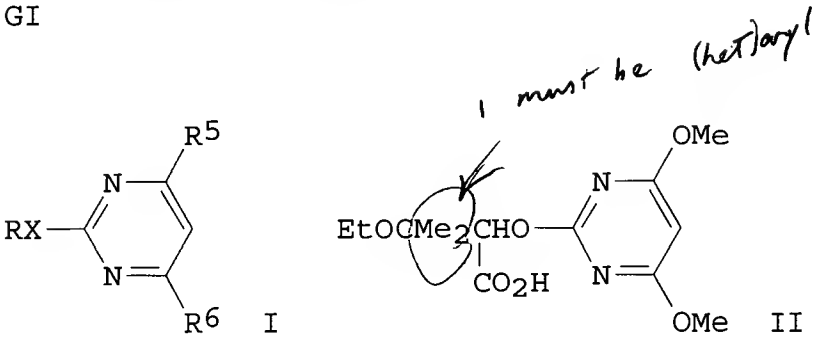
AB The title compds. [I; R1 = H, succinimidyloxy residue, (un)substituted N-contg. 5-membered heterocyclic residue, etc.; R2, R3 = halogen, alkyl, alkoxy, thioalkyl, etc.; R4 = C1-10 alkyl contg. 1-5 halogen atom(s), (un)substituted heterocyclyl residue, (un)substituted Ph or naphthyl, etc.; R5 = H, alkyl, alkenyl, alkynyl, cycloalkyl, etc.; R6 = (un)substituted Ph or naphthyl, (un)substituted heteroaryl, etc.; X = undefined (sic); Y = direct bond, O, S; Z = S, O] (e.g., R1-R3 = OMe, R4 = R6 = Ph, R5 = Me, X = CH, Y = Z = O; m.p. 100-103.degree.), useful as agrochem. herbicides for the control of unwanted plants in crop fields, are prepd. and a I-contg. formulation presented.

IT **159308-02-8P**
RL: AGR (Agricultural use); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 3-(hetero)aryloxy(thio)carboxylic acid derivs. as

agrochem. herbicides)
IT **159308-03-9P 159308-04-0P 159308-05-1P**
159308-06-2P 159308-07-3P 159308-08-4P
159308-09-5P 159308-10-8P 159308-11-9P
159308-12-0P 159308-13-1P 159308-14-2P
159308-15-3P 159308-16-4P 159308-17-5P
159308-18-6P 159308-19-7P
RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 3-(hetero)aryloxy(thio)carboxylic acid derivs. as agrochem. herbicides)
IC ICM C07D239-60
ICS C07D251-26; C07D405-12; C07D409-12; C07D491-048; C07D403-12; C07D417-12; C07D413-12; C07D413-14; C07D401-12; A01N043-54; A01N043-66
ICA C07D521-00; C07D333-24; C07D307-54
ICI C07D405-12, C07D239-60, C07D251-26, C07D307-54; C07D409-12
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 5
IT **159308-02-8P**
RL: AGR (Agricultural use); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 3-(hetero)aryloxy(thio)carboxylic acid derivs. as agrochem. herbicides)
IT **159308-03-9P 159308-04-0P 159308-05-1P**
159308-06-2P 159308-07-3P 159308-08-4P
159308-09-5P 159308-10-8P 159308-11-9P
159308-12-0P 159308-13-1P 159308-14-2P
159308-15-3P 159308-16-4P 159308-17-5P
159308-18-6P 159308-19-7P
RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 3-(hetero)aryloxy(thio)carboxylic acid derivs. as agrochem. herbicides)

L9 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 1996 ACS
AN 1992:448600 HCAPLUS
DN 117:48600
TI Preparation of 3-alkoxy-2-pyrimidyloxy- and -thioalkanoates as herbicides
IN Harada, Katsumasa; Abe, Takaaki; Akiyoshi, Yuji; Shiraishi, Hiroshi; Yamamoto, Kaoru
PA Ube Industries, Ltd., Japan
SO Eur. Pat. Appl., 65 pp.
CODEN: EPXXDW
PI EP 481512 A1 920422
DS R: DE, FR, GB, IT
AI EP 91-117829 911018

PRAI JP 90-279328 901019
JP 91-189613 910423
DT Patent
LA English
OS MARPAT 117:48600
GI



AB Title compds. [I; R = R1OCR2R3CH(CO2R4); R1 = (cyclo)alkyl, alkenyl, alkynyl, haloalkyl, cyanoalkyl; R2 = H, alkyl; R3 = (cyclo)alkyl; R2R3 = atoms to complete a carbocyclic ring; R4 = H, alkyl, alkynyl; R5 = (halo)alkyl, alkoxy, halo; R6 = alkyl, alkoxy; X = O, S] were prepd. Thus, Et 2,3-epoxy-3-methylbutanoate was treated with H2SO4 in EtOH and the product condensed with 4,6-dimethoxy-2-methylsulfonylpyrimidine to give, after sapon., title compd. II which gave complete control of 5 weeds, e.g., crabgrass, with slight damage to cotton at 20 g/are preemergent.

IT **142411-65-2P 142411-66-3P 142411-99-2P**
142412-00-8P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as herbicide)

IC ICM C07D239-60
ICS C07D239-52; C07D239-34; A01N043-54

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 5

IT 134433-11-7P 134433-27-5P 142411-45-8P 142411-46-9P
142411-47-0P 142411-48-1P 142411-49-2P 142411-50-5P
142411-51-6P 142411-52-7P 142411-53-8P 142411-54-9P
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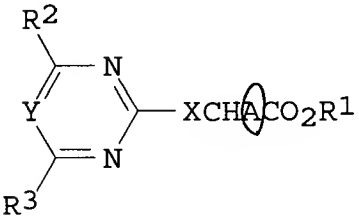
142430-13-5P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as herbicide)

L9 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 1996 ACS
AN 1991:429369 HCAPLUS
DN 115:29369
TI Preparation of 2-aryl-2-(2-pyrimidinyloxy)acetates and analogs as agrochemicals
IN Wegner, Peter; Harde, Christoph; Nordhoff, Erhard; Krueger, Anita; Krueger, Gabriele; Tarara, Gerhard; Heinrich, Nikolaus; Rees, Richard; Johann, Gerhard; Koetter, Clemens
PA Schering A.-G., Fed. Rep. Ger.
SO Eur. Pat. Appl., 26 pp.
CODEN: EPXXDW
PI EP 409368 A2 910123

DS R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE
AI EP 90-250184 900719
PRAI DE 89-3924259 890719
DE 90-4009481 900322
DT Patent
LA German
OS MARPAT 115:29369
GI



I

AB The title compds. [I; A = (halo)alkyl, alkenyl, cycloalkyl, PhCH2, (un)substituted Ph, pyridyl, naphthyl, etc.; R1 = H, alkyl, PhCH2; R2, R3 = alkyl, alkoxy, alkylthio, (di)alkylamino, halo; X = O, S; Y = CH, N] were prepd. as agrochem. fungicides, herbicides, and plant growth regulators. Thus, MeSO2OR (R = 4,6-dimethoxypyrimidinyl) was condensed with HSCH2CO2Me and the product condensed with CH2:CHCH2Br to give CH2:CHCH2CH(OR)CO2Me. ROCHPhCO2Me gave 75-89% control of 5 weeds (e.g. Abutilon theophrasti) at 1.0 kg/ha postemergent.

IT **134433-24-2P 134461-60-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as agrochem.)

IC ICM C07D239-60
ICS C07D401-12; C07D251-30; C07D251-38; C07D403-12; C07D405-12; C07D409-12; C07D251-46; A01N043-54; A01N043-66

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 5

IT 127091-57-0P 127091-63-8P 127091-73-0P 127091-77-4P
127091-78-5P 133458-29-4P 133458-30-7P 133458-32-9P
133458-34-1P 133483-96-2P 133483-97-3P 134432-62-5P
134432-63-6P 134432-64-7P 134432-65-8P 134432-66-9P
134432-67-0P 134432-68-1P 134432-69-2P 134432-70-5P
134432-71-6P 134432-72-7P 134432-73-8P 134432-74-9P
134432-75-0P 134432-76-1P 134432-77-2P 134432-78-3P
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134432-83-0P 134432-84-1P 134432-85-2P 134432-86-3P
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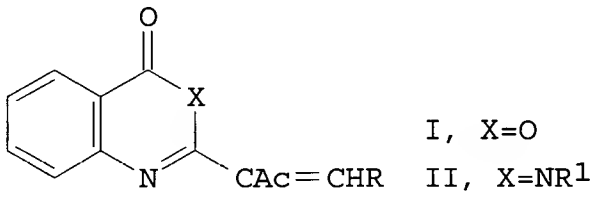
134433-19-5P 134433-20-8P 134433-21-9P 134433-22-0P
134433-23-1P **134433-24-2P** 134433-25-3P 134433-26-4P
134433-27-5P 134433-28-6P 134461-59-9P **134461-60-2P**
134461-61-3P 134461-62-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as agrochem.)

L9 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 1996 ACS
AN 1981:515443 HCAPLUS
DN 95:115443
TI Synthesis and reactions of 2-(.alpha.-acetylstyryl)-3,1-benzoxazin-(4H)-ones and 2-(.alpha.-acetylstyryl)-quinazolin-4-(3H)-ones
AU Elkasaby, M. A.; Noureldin, N. A.
CS Fac. Sci., Ain Shams Univ., Cairo, Egypt
SO Indian J. Chem., Sect. B (1981), 20B(4), 290-3
CODEN: IJSBDB; ISSN: 0376-4699
DT Journal
LA English
GI



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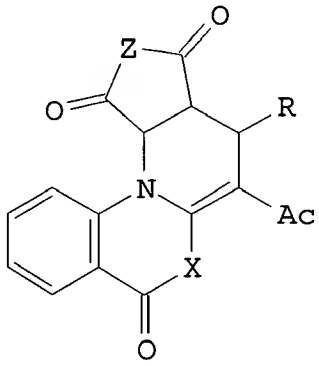
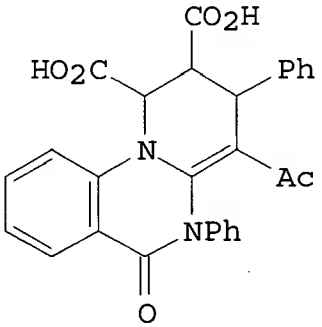
II, X=NR1



III, X=Z=O
IV, X=NR1, Z=O
VI, X=O, Z=PhN
VII, X=NR1, Z=PhN



V

AB Benzoxazinones I (R = Ph, p-MeOC6H4, p-Me2NC6H4) and quinazolines II (R = Ph, p-MeOC6H4; R1 = H, Ph, p-MeC6H4, p-MeOC6H4) were prepd. from o-HO2CC6H4NHCOCAc:CHR. I (R = Ph, p-MeOC6H4) react with maleic anhydride to give furopyridobenzoxazines III. Several II similarly underwent Diels-Alder reaction with maleic anhydride to give the furopyridoquinazolines IV. IV (R = R1 = Ph) was hydrolyzed to give the pyridoquinazoline V. II and III reacted with N-phenylmaleimide to give cycloadducts VI and VII, resp. Reaction of I with Grignard reagent and II with PhSH were investigated.

IT **78817-76-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))

IT 70723-69-2P 78817-52-4P 78817-55-7P 78817-56-8P 78817-57-9P
78817-58-0P 78817-60-4P 78817-61-5P 78817-62-6P 78817-63-7P
78817-64-8P 78817-65-9P 78817-66-0P 78817-67-1P 78817-68-2P
78817-69-3P 78817-70-6P 78817-71-7P 78817-72-8P 78817-73-9P
78817-74-0P 78817-75-1P **78817-76-2P** 78817-77-3P
78817-78-4P 78817-79-5P 78834-04-5P 78852-97-8P 78922-69-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

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FILE 'REGISTRY' ENTERED AT 07:43:57 ON 05 SEP 96
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STRUCTURE FILE UPDATES: 02 SEPT 96 HIGHEST RN 180310-23-0
DICTIONARY FILE UPDATES: 04 SEPT 96 HIGHEST RN 180310-23-0

TSCA INFORMATION NOW CURRENT THROUGH DECEMBER 1995

Please note that search-term pricing does apply when conducting SmartSELECT searches.

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(159559-11-2/RN)
1 159559-24-7/BI
(159559-24-7/RN)
1 170296-16-9/BI
(170296-16-9/RN)
1 170296-36-3/BI
(170296-36-3/RN)
1 170296-42-1/BI
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1 170296-44-3/BI
(170296-44-3/RN)
1 170296-46-5/BI

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                OR 170296-77-2/BI OR 170296-79-4/BI OR 170296-81-8/BI OR 1
                70296-82-9/BI)

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L10  ANSWER 1 OF 17  REGISTRY  COPYRIGHT 1996 ACS
RN   170296-82-9  REGISTRY
CN   Benzenepropanoic acid, .alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-
     .beta.-[(3-fluorophenyl)methoxy]-.beta.-methyl-, sodium salt (9CI)
     (CA INDEX NAME)
MF   C23 H23 F N2 O6 . Na
SR   CA
LC   STN Files:   CA, CAPLUS, TOXLIT
CRN  (170296-81-8)
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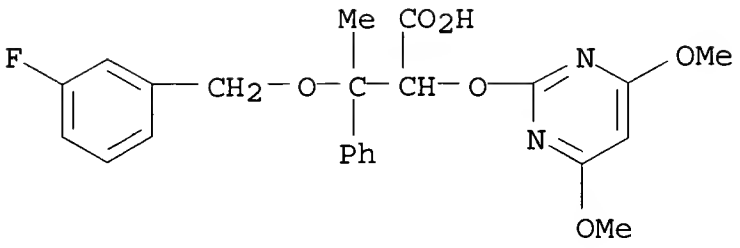
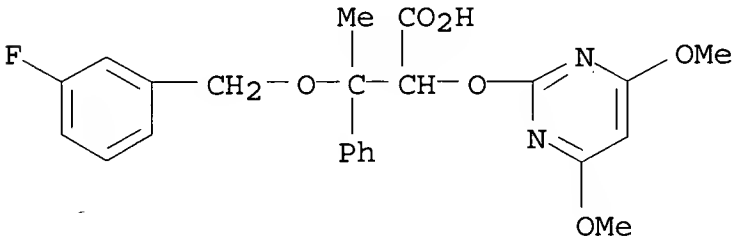


● Na

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:307319

L10 ANSWER 2 OF 17 REGISTRY COPYRIGHT 1996 ACS
RN **170296-81-8** REGISTRY
CN Benzenepropanoic acid, .alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-.beta.-[(3-fluorophenyl)methoxy]-.beta.-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H23 F N2 O6
CI COM
SR CA
LC STN Files: CA, CAPLUS, TOXLIT

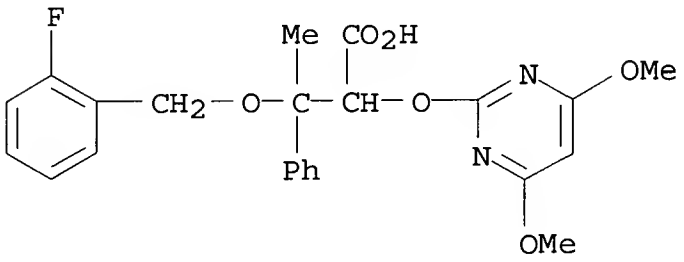


1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:307319

L10 ANSWER 3 OF 17 REGISTRY COPYRIGHT 1996 ACS
RN **170296-79-4** REGISTRY

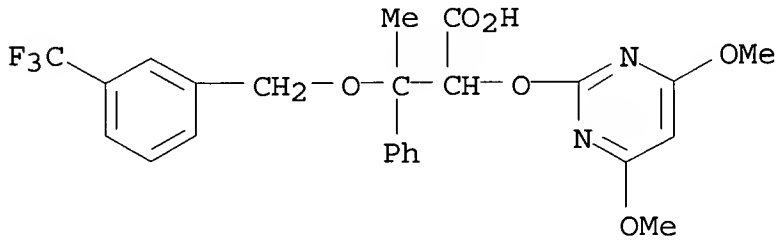
CN Benzenepropanoic acid, .alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-.beta.-[(2-fluorophenyl)methoxy]-.beta.-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H23 F N2 O6
SR CA
LC STN Files: CA, CAPLUS, TOXLIT



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:307319

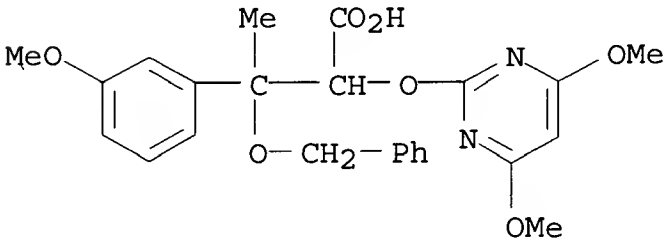
L10 ANSWER 4 OF 17 REGISTRY COPYRIGHT 1996 ACS
RN **170296-77-2** REGISTRY
CN Benzenepropanoic acid, .alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-.beta.-methyl-.beta.-[[3-(trifluoromethyl)phenyl]methoxy]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C24 H23 F3 N2 O6
SR CA
LC STN Files: CA, CAPLUS, TOXLIT



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:307319

L10 ANSWER 5 OF 17 REGISTRY COPYRIGHT 1996 ACS
RN **170296-72-7** REGISTRY
CN Benzenepropanoic acid, .alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-3-methoxy-.beta.-methyl-.beta.-(phenylmethoxy)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C24 H26 N2 O7
SR CA
LC STN Files: CA, CAPLUS, TOXLIT



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:307319

L10 ANSWER 6 OF 17 REGISTRY COPYRIGHT 1996 ACS
RN **170296-60-3** REGISTRY
CN Benzenepropanoic acid, .beta.-[(4-chlorophenyl)methoxy]-.alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-.beta.-methyl- (9CI) (CA INDEX NAME)
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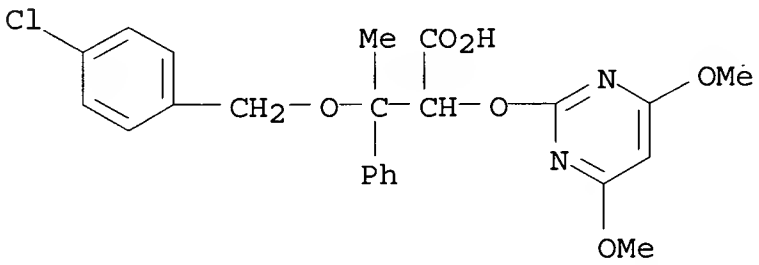
SR CA
LC STN Files: CA, CAPLUS, TOXLIT



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:307319

L10 ANSWER 7 OF 17 REGISTRY COPYRIGHT 1996 ACS
RN **170296-54-5** REGISTRY
CN Benzenepropanoic acid, .alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-.beta.-ethyl-.beta.-(phenylmethoxy)- (9CI) (CA INDEX NAME)
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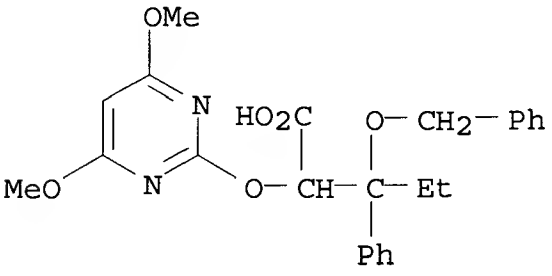
SR CA
LC STN Files: CA, CAPLUS, TOXLIT



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1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:307319

L10 ANSWER 8 OF 17 REGISTRY COPYRIGHT 1996 ACS
RN **170296-52-3** REGISTRY
CN Benzenepropanoic acid, .alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-.beta.,4-dimethyl-.beta.-(phenylmethoxy)- (9CI) (CA INDEX NAME)
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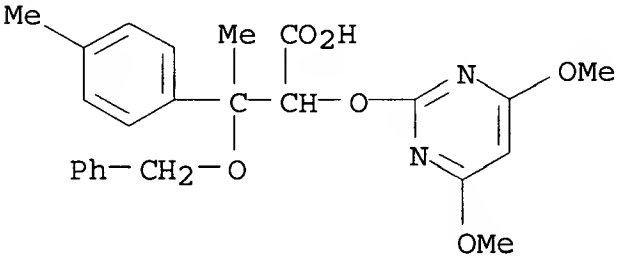
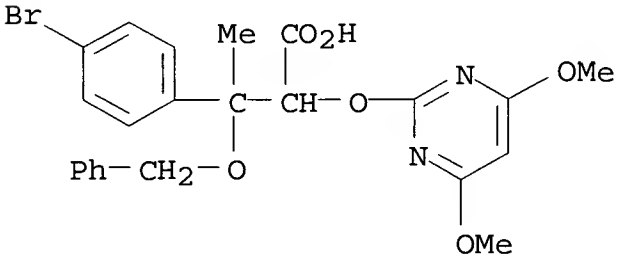
SR CA
LC STN Files: CA, CAPLUS, TOXLIT



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:307319

L10 ANSWER 9 OF 17 REGISTRY COPYRIGHT 1996 ACS
RN **170296-50-1** REGISTRY
CN Benzenepropanoic acid, 4-bromo-.alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-.beta.-methyl-.beta.-(phenylmethoxy)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H23 Br N2 O6
SR CA
LC STN Files: CA, CAPLUS, TOXLIT



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1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:307319

L10 ANSWER 10 OF 17 REGISTRY COPYRIGHT 1996 ACS
RN **170296-48-7** REGISTRY
CN Benzenepropanoic acid, .alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-2-fluoro-.beta.-methyl-.beta.-(phenylmethoxy)- (9CI) (CA INDEX NAME)
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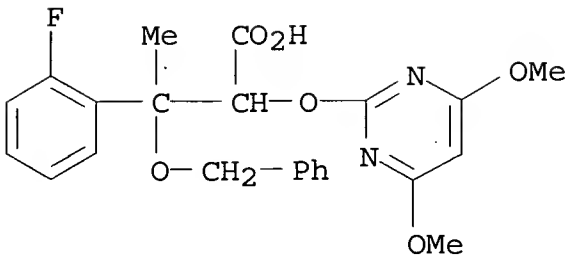
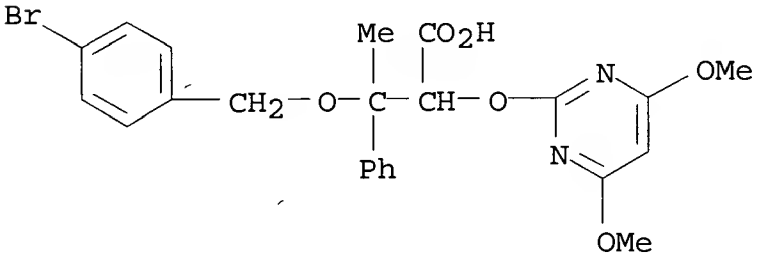
SR CA
LC STN Files: CA, CAPLUS, TOXLIT



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:307319

L10 ANSWER 11 OF 17 REGISTRY COPYRIGHT 1996 ACS
RN **170296-46-5** REGISTRY
CN Benzenepropanoic acid, .beta.-[(4-bromophenyl)methoxy]-.alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-.beta.-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H23 Br N2 O6
SR CA
LC STN Files: CA, CAPLUS, TOXLIT

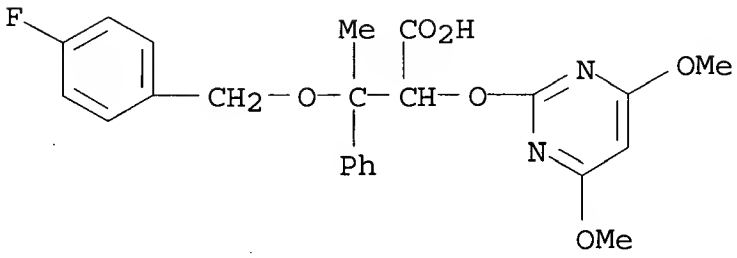


1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:307319

L10 ANSWER 12 OF 17 REGISTRY COPYRIGHT 1996 ACS
RN **170296-44-3** REGISTRY
CN Benzenepropanoic acid, .alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-.beta.-[(4-fluorophenyl)methoxy]-.beta.-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H23 F N2 O6
SR CA

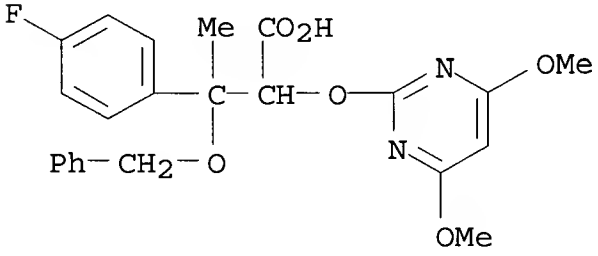
LC STN Files: CA, CAPLUS, TOXLIT



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:307319

L10 ANSWER 13 OF 17 REGISTRY COPYRIGHT 1996 ACS
RN **170296-42-1** REGISTRY
CN Benzenepropanoic acid, .alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-4-fluoro-.beta.-methyl-.beta.-(phenylmethoxy)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H23 F N2 O6
SR CA
LC STN Files: CA, CAPLUS, TOXLIT

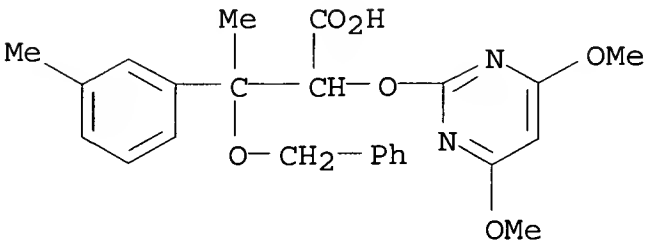


1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:307319

L10 ANSWER 14 OF 17 REGISTRY COPYRIGHT 1996 ACS
RN **170296-36-3** REGISTRY
CN Benzenepropanoic acid, .alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-.beta.,3-dimethyl-.beta.-(phenylmethoxy)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C24 H26 N2 O6

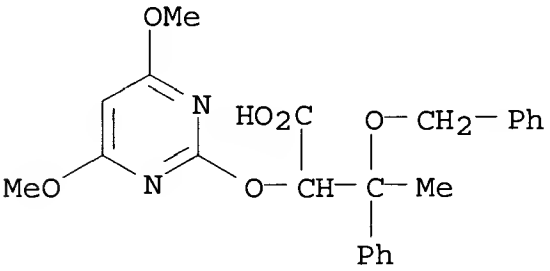
SR CA
LC STN Files: CA, CAPLUS, TOXLIT



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:307319

L10 ANSWER 15 OF 17 REGISTRY COPYRIGHT 1996 ACS
RN **170296-16-9** REGISTRY
CN Benzenepropanoic acid, .alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-.beta.-methyl-.beta.-(phenylmethoxy)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H24 N2 O6
SR CA
LC STN Files: CA, CAPLUS, TOXLIT



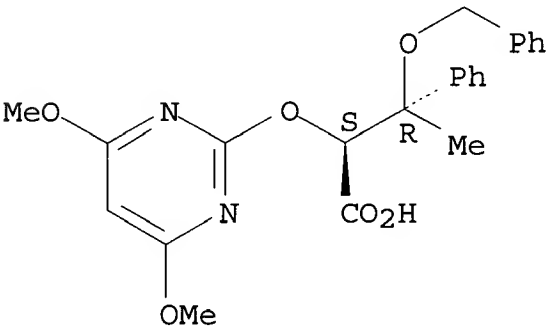
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:307319

L10 ANSWER 16 OF 17 REGISTRY COPYRIGHT 1996 ACS
RN **159559-24-7** REGISTRY
CN Benzenepropanoic acid, .alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-.beta.-methyl-.beta.-(phenylmethoxy)-, (R*,S*)- (9CI) (CA INDEX

NAME)
FS STEREOSEARCH
MF C23 H24 N2 O6
SR CA
LC STN Files: CA, CAPLUS
DES 2:R*,S*

Relative stereochemistry.

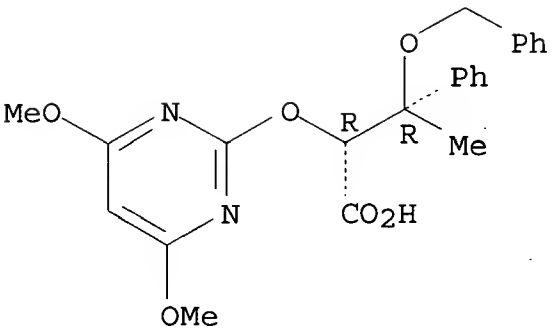


1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 122:31550

L10 ANSWER 17 OF 17 REGISTRY COPYRIGHT 1996 ACS
RN **159559-11-2** REGISTRY
CN Benzenepropanoic acid, .alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-.beta.-methyl-.beta.-(phenylmethoxy)-, (R*,R*)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C23 H24 N2 O6
SR CA
LC STN Files: CA, CAPLUS
DES 2:R*,R*

Relative stereochemistry.



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 122:31550

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